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This is a final report on research performed, under AFOSR Grant-87-0284 for the period 1 June 1987 to 31 May 1988, on microstructural dynamics of particulate and granular media. Methods of statistical physics have been applied to the interpretation of computer simulations of the mechanical and transport properties granular materials and disordered solids. A new continuum theory of Reynolds dilatancy in granular masses has been developed and a mechanical test facility has been developed under joint funding from the National Science Foundation.

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FINAL REPORT

on

RESEARCH

AFOSR-TR- 88-1155

CRITICAL BEHAVIOR OF TRANSPORT AND MECHANICAL PROPERTIES IN PARTICULATE DISPERSIONS AND GRANULAR MEDIA

performed under

AFOSR Grant-87-0284

for the period

1 June 1987 - 31 May 1988

Submitted by

J. D. Goddard, J. P. Bardet, C. Campbell and M. Sahimi
Principal Investigators
University of Southern California

to

Major Steven C. Boyce
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Directorate of Aerospace Sciences
Department of Air Force
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29 July 1988

CRITICAL BEHAVIOR OF TRANSPORT AND MECHANICAL PROPERTIES IN PARTICULATE DISPERSIONS AND GRANULAR MEDIA

RESEARCH SUMMARY

This is the final report on a one year research activity supported in part by AFOSR Grant - 87-0284 for the period 1 June 1987 to 31 May 1988. This work is part of an on-going program of theoretical and experimental research on the microstructural dynamics and continuum mechanics of concentrated particulate dispersions and granular materials which is supported also by the National Science Foundation (NSF). Particular emphasis is devoted to the study of mechanical and scalar transport properties in the regime of yielding and incipient flow. The intent is to bring various techniques from modern statistical physics to bear on the problem of extracting effective-continuum models from micromechanical theories. The goal is to improve modeling and prediction of mechanical and scalar-transport properties and of microstatistical failure and deformation processes in soils, particulate media and more general materials. The present effort involves an interdisciplinary team of researchers in the University of Southern California School of Engineering, which combines expertise in soil mechanics, granular materials, statistical physics, molecular transport phenomena, continuum mechanics and rheology.

Following is a report on the first-year activity. As a complement to the research activity cited below, we are conducting bi-weekly seminars, involving about ten to fifteen persons from Ch.E., C.E. and M.E. as well as outside speakers.

Appended is a summary of publications and talks related to the present grant activity.

I. COLLABORATIVE RESEARCH EFFORTS.

A. Experiments and theoretical modeling of the quasi-static mechanics in 2-d ("Schneebli") assemblages.

1. Experiments on 2-d optical-fibers arrays

J. D. Goddard (Ch.E.) and J. P. Bardet (C.E.) have worked with two M.S. students, one in Ch.E. and one in C.E., on development of experimental measurements of both stress and displacement in bundles of optical fibers.

Following previous investigations [1], [2], we plan to use photoelastic measurements of stress, employing an optical birefringence facility available in the Ch.E. Department (and provided by a prior NSF equipment grant). In our work, 0.5 mm diameter optical-quality glass fibers chopped to a uniform length (approx. 2 cm), allow for small overall sample dimensions (2 cm square cross section), relatively inexpensive loading device and high quality optical transmission. Figure 1 provides photographs of the mechanical test facility (photoelastic facility not included).

In addition we wish to follow particle displacements and, for this purpose, we are developing a PC-based video-image acquisition/analysis system combined with a photochromic tracer technique, based on equipment provided by the NSF grant. As one goal, we hope to analyze phenomena such as "bridging" or "arching" in granular assemblies. See Figure 2.

2. Numerical simulation of the quasi-static mechanics of 2-d particle assemblies disks or cylinders).

J. D. Goddard and M. Sahimi (Ch.E.) are working with a Ph.D. student (in Ch.E.) on the modeling of particle motion and force distribution in 2-d assemblies of stiff elastic particles with coulombic-frictional contacts. For this purpose, we are employing an NSF grant of time on CRAY-XMP at the San Diego Supercomputer Center, consisting of 75 units in 1987-88 and a renewal grant of 100 units for 1988-89.

Besides being somewhat simpler theoretically, 2-d assemblies provide a testing ground for statistical-physics theories involving variable spatial dimension. As one question, we ask whether the bridging or force-channeling evident in Figure 2 represents a "percolation" phenomenon.

We have been able to follow the quasi-static motion of 100-particle assemblages through macroscopic strains of a fifty percent or more. A forthcoming paper by J. D. Goddard and Y. Bashir will employ some of these results in a new continuum theory of Reynolds dilatancy in granular masses. Ultimately, we intend to compare more extensive computations with experiments, both ours and those of others, on granular masses.

Dr. Bardet has recently proposed to Dr. Matsuoka of the Nagoya Institute, Japan, a collaborative program of research in the area (see appended letter), with one long-term goal being the micromechanical elucidation of the seismic liquefaction of soils.

B. Diffusional (scalar) transport properties and mechanics of dense particle suspensions.

J. D. Goddard (Ch.E.) and C. S. Campbell (M.E.) are working with graduate research assistants in Ch.E. and M.E. on various experimental aspects of thermal or electrical conductivity in static and flowing suspensions. As one major accomplishment, we have developed in the summer of 1987 an ionically-conducting particle suspension, consisting of a ionically-doped anion-exchange resin. As an electrolyte, this suspension can behave either as a large-Peclet number (convection-dominated) transport system for a (DC) electrochemical redox reaction, or else as a zero-Peclet number (conduction-dominated) system, for total (AC) ionic conductivity. Employing a rotating-disk electrode in the Ch.E. laboratories, we have gathered extensive data to characterize this system, as an extension of the works of References [3] and [4].

Figure 3 shows typical data collected on a suspension of ion-exchange resin above the rotating-disk electrode (cf. [4]). At present, we are designing a shear cell, to determine simultaneously the shear stress and conductivity in such suspensions.

II. RELATED STUDIES AND CONTINUATION.

In addition to the above collaborative research the P.I.'s are independently pursing research in the following areas:

A. **Rapid flow of granular media** (C. S. Campbell, M.E.)

B. **Continuum-models and mechanics of failure processes in geomaterials: strain-localization, spalling, etc.** (J. P. Bardet, C.E.)

C. **Statistical physics of disordered elastic systems** (M. Sahimi, Ch.E.)

The subject AFOSR grant has been most helpful in assuring a vigorous start-up of our collaborative research effort during the first year.

We believe the scope and accomplishments of the work underway merits continued AFOSR support, and we expect to submit a proposal for such in the near future.

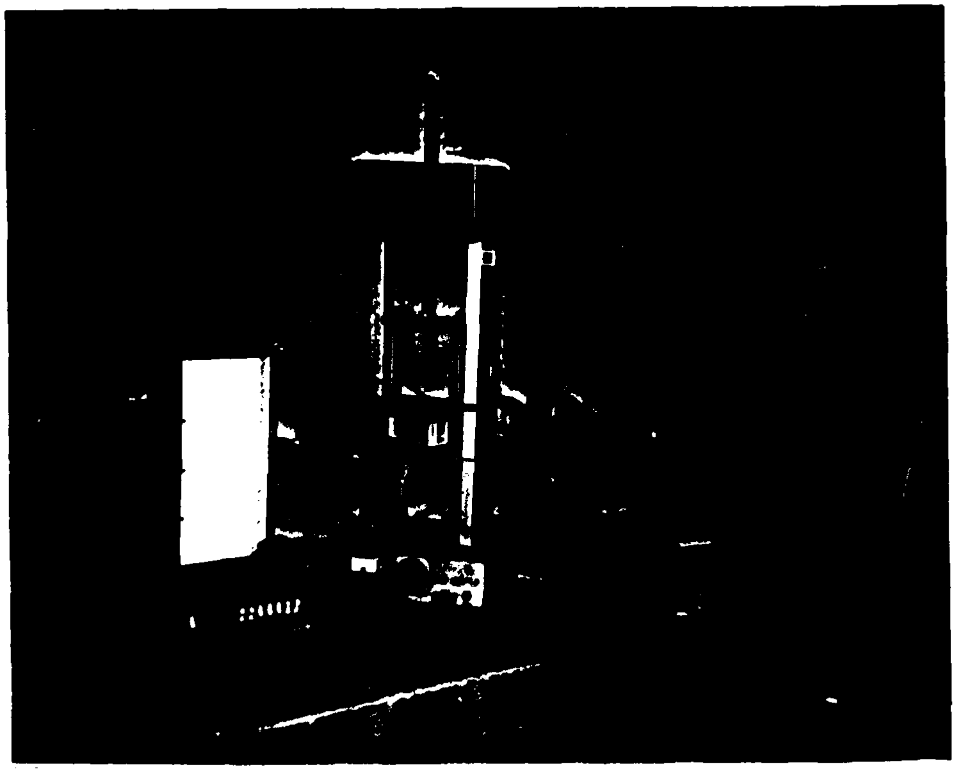
REFERENCES

1. Matsuoka, H., "Deformation and Strength of Granular Materials Based on the Theory of "Compound Mobilized Planes" (CMP) and "Spatial Mobilized Planes" (SMP), *in* Vol. II of Advances in the Mechanics and the Flow of Granular Materials (M. Shahinpoor, Ed.) Trans. Tech./Gulf Publishing Co., 1983.

2. Supel, J. A., "Local Destruction of Granular Media Caused by Crushing a Single Grain", *Arch. Mech.*, **37**, 535 (1985).

3. Turner, J.C.R., "Two-Phase Conductivity - the Electrical Conductivity of Liquid-fluidized beds of Spheres", *C.E.S.*, **31**, 487 (1976).

4. Muller, R. H., Roha, D. J., and Tobias, C. W., "Effect of Suspended Particles on the Rate of Mass Transfer to a Rotating Disk Electrode", *in* "Transport Processes in Electrochemical Systems", (R. S. Yeo, T. Katam and D.-T. Chin, eds.) Proceeding Electrochem. Soc., Vo. 82-10, pp. 1-15, 1982.



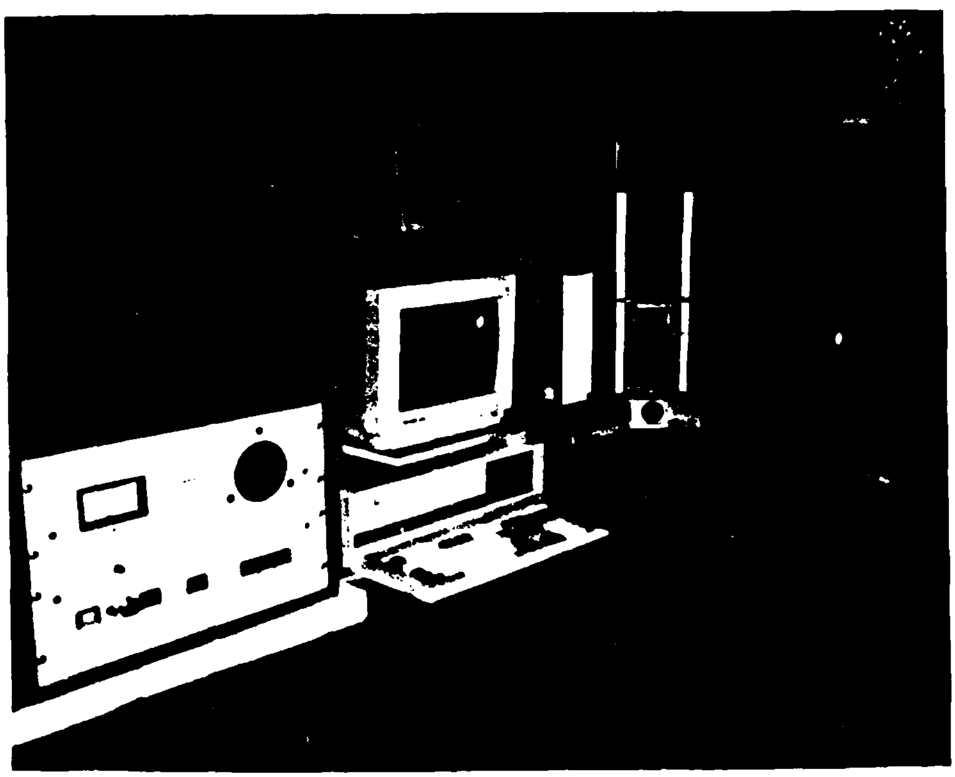


Figure 1. Components of mechanical test facility. Upper photo.: (left to right) Pulsed-UV lamp, compression tester and load cell, video camera and monitor for digital image. Lower photo.: Larger view, including power supply for UV lamp and PC employed to digitize and analyze images.

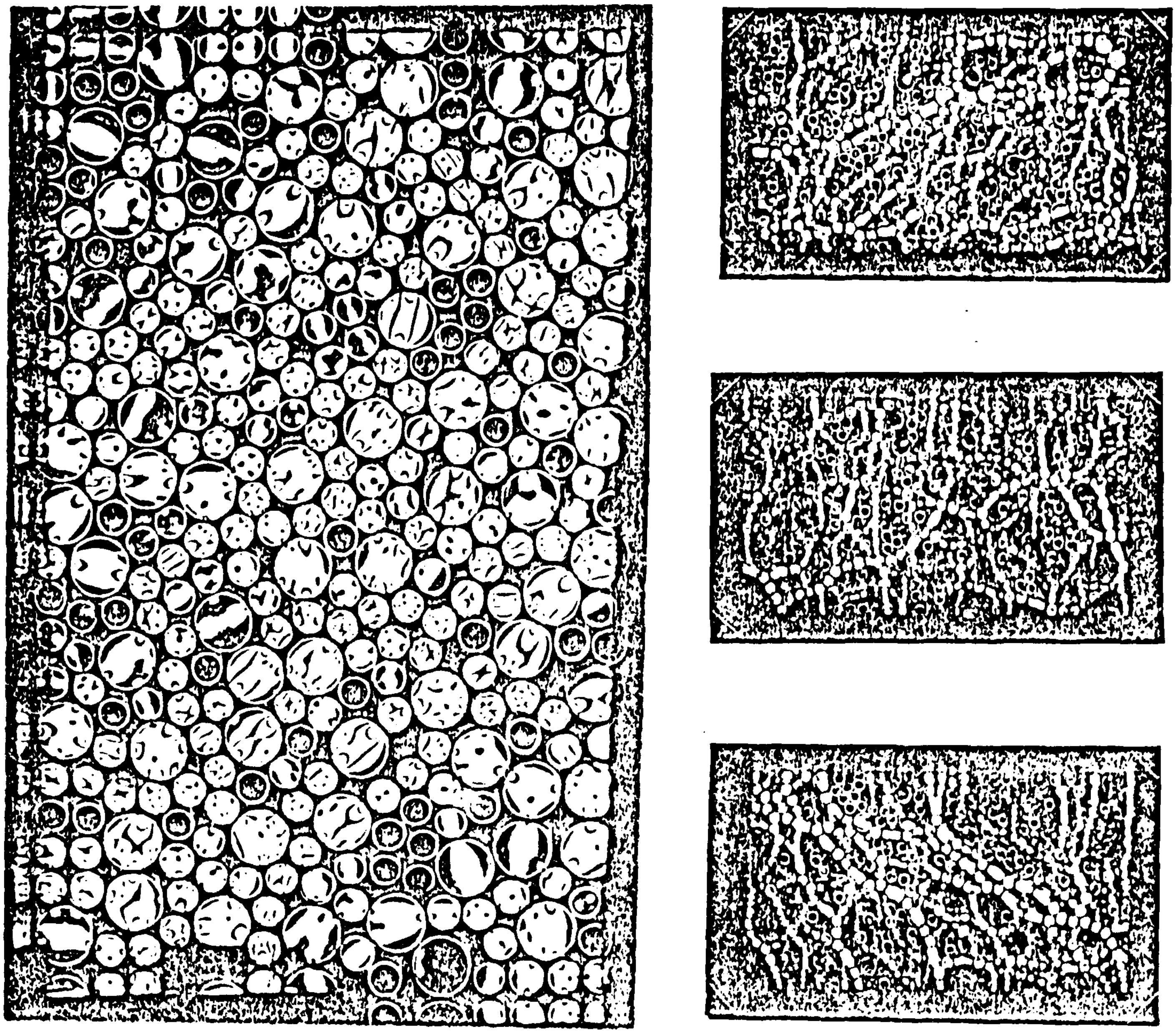


Figure 2. Photoelastic birefringence patterns in plastic (araldite-B) rod bundles. (a) close-up of fringe-pattern (b) illuminated force-chains, show bridging ("percolation"?) phenomenon under three different states of loading. (Courtesy of Prof. H. Matsuoka, Nagoya Institute of Technology: Private communication to J.P. Bardet.)

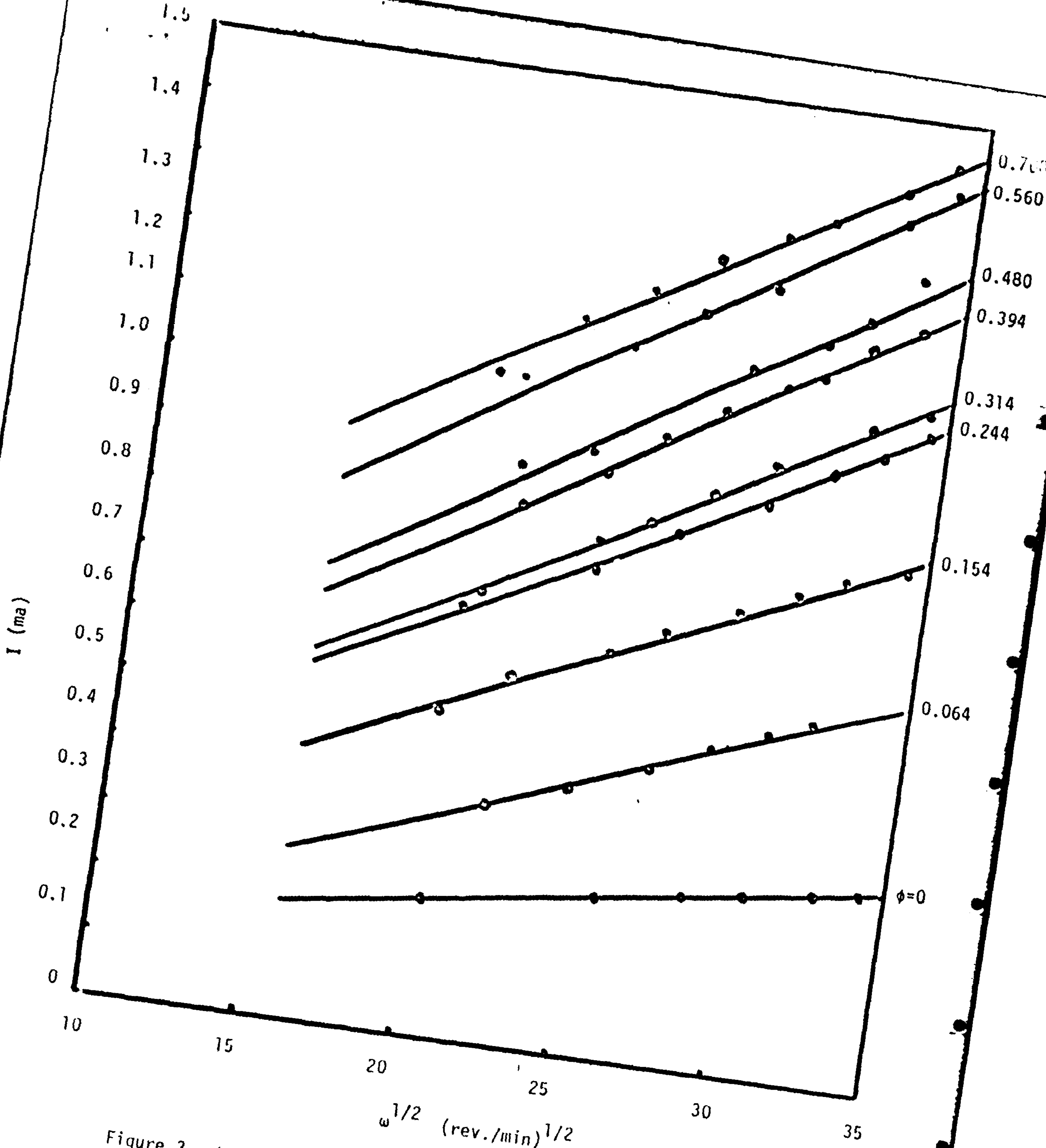


Figure 3. Limiting current I for Ferricyanide reduction on rotating disk cathode vs. square root of disk rotation speed ω at various suspension volume-fractions ϕ of anion ion-exchange resin beads (550μm diameter.)

PUBLICATIONS AND TALKS BY J. P. BARDET

Related to Present Research

I. Conference Papers and Invited Talks:

"A Numerical Approach of Strain Localization and Rockburst", seminar at the Ecole Centrale de Paris, Paris, France, 19 June 1987.

"Finite Element Modelling of Strain Localization", seminar at the Institut de Mecanique de Grenoble, France, 23 June 1987.

"Finite Element Modelling of Rockburst", seminar at the Institut de Mecanique de Grenoble, France, 26 June 1987.

"Numerical Simulation of Strain Localization During Plane Strain Compression of Over-consolidated Clay", presented at the 6th Specialty Conference of the American Society of Civil Engineers, Engineering Mechanics Division, State University of New York at Buffalo, 21 May 1987.

"Strain Localization in Dense Soils", seminar at the City University, London, U.K., 2 July 1987.

"A Note on the Finite Element Modeling of Strain Localization", paper by J. P. Bardet presented at the International Conference NUMETA, Swansea, Wales, 7 July 1987.

"Modelling of Strain Localization and Surface Instability in Geomechanics", seminar of the Civil Engineering Department at the University of Arizona, 30 October 1987.

"Research in Geomechanics at the University of Southern California", lecture in Nagoya organized by Japanese Society of Soil Mechanics and Foundation, Japan, 4 December 1987.

"Strain Localization and Surface Instability", seminar at Kyoto University, Japan, 7 December 1987.

II. Papers Accepted and Submitted for Publication:

"Finite Element Analysis of Surface Instability in Hypo-Elastic Solids", submitted to *Computer Methods in Appl. Mech. & Eng.*, 1988.

PUBLICATIONS AND TALKS BY C. S. CAMPBELL

Related to Present Research

I. Conference Papers and Invited Talks:

"Computer Simulation of Rapid Granular Flow Kinetic Theories for Planetary Rings", Seminar, Cornell University, Cornell University, May 1987.

"Boundary Conditions for Two-dimensional Granular Flow", Sino-US Symposium on Multiphase Flows, Hangzhou, China, August, 1987.

"A Technique for Determining the Fluidization Mechanism in Horizontal Slurry Flow", DOE Advanced Solids Transport Contractor's Meeting, Pittsburgh, PA, September 1987.

"Boundary Interactions for Two-dimensional Granual Flows: Asymmetric Stresses and Couple Stresses", Proc. US-Japan Seminar on the Micromechanics of Granular Material, Sendai-Zao, Japan, October 1987.

II. Papers Accepted and Submitted for Publication:

"Self Lubrication for Long Runout Landslides" accepted for publication in *J. Geol.* (1988).

"Boundary Interactions for Two-dimensional Granual Flows: Asymmetric Stresses and Couple Stresses", Proc. US-Japan Seminar on the Micromechanics of Granular Material, Sendai-Zao, Japan, October 1987..

"Particle Rotation as a Heat Transfer Mechanism", submitted to *Intl. J. Heat and Mass Transfer (1988).*

PUBLICATIONS AND TALKS BY J. D. GODDARD

Related to Present Research

I. Conference Papers and Invited Talks:

"Monte-Carlo Simulations of Shear Flow of Granular Media", March Meeting of American Physical Society, NY, March 16-20, 1987. Abstract in *Bull. Am. Phys. Soc.*, **32** (3) 732 (1987). (With Y. Bashir and M. Sahimi)

"Microstructural Models for Slow Deformations of Dense Granular Dispersions", Engineering Foundation Conference on Fluid Particle Interactions, Davos, Switzerland, May 3-8, 1987.

"Rheology of Dense Particulate Dispersions and Granular Media" (Invited Paper), A.I.Ch.E. Conference on Emerging Technologies in Materials, paper P3.1, Minneapolis, MN, Aug. 10-18, 1987.

"Mechanical and Transport Properties of Granular Media", AFOSR Seminar on Soil Mechanics, M.I.T., Boston, MA, Sept. 14-15, 1987.

"Continuum and Microstructural Models for Dilatancy in Granular Masses", presented at the March Meeting of American Physical Society, New Orleans, March 20-25, 1988 (Focussed Session on Granular Materials, co-organized by Dr. Peter Haff, Caltech, and P.I., J. D. Goddard) and as a graduate seminar in Applied Mathematics, U. Western Ontario, London, Ontario, Canada, June 27, 1988. Abstract in *Bull. Am. Phys. Soc.*, **33**, 799 (1988).

"Force Percolation, Dilatancy, Yield and Strain Localization in Granular Media", 19th Ann. Mtg. Fine Particle Society, Santa Clara, CA, July 19-22, 1988. (with Y. Bashir)

"Continuum and Microstructural Models for Dilatancy in Granular Fluids", accepted for presentation in sessions, Fundam. Research in Fluid Dynamics Ann. A.I.Ch.E. Mtg., Washington, D.C., Nov. 27-Dec. 2, 1988. (with Y. Bashir).

PUBLICATIONS AND TALKS BY M. SAHIMI

Related to Present Research

I. Conference Papers and Invited Talks:

"Computer Simulations of Linear and Nonlinear Transport Processes in Disordered Solids", Department of Chemical Engineering, University of California, San Diego, September 30, 1987.

"Computer Simulations of Linear and Nonlinear, Scalar and Vector Transport Processes in Disordered Media", Department of Chemical Engineering, Universisty of California Los Angeles, February 5, 1988.

"Statistical Physics of Linear and Nonlinear, Scalar and Vector Transport Processes in Disordered Media", Third University of California Conference on Statistical Mechanics, Davis, March 27-30, 1988.

II. Papers Accepted and Submitted for Publication:

"Distribution of Fracture Strengths in Disordered Continua", *Phys. Rev.*, **B36,** 8656 (1987). (with M. D. Stephens)

"Absence of Universality in Percolation Models of Disordered Elastic Media with Central Forces", *Journal of Physics A,* in press (1988). (with S. Arbabi)

"Elastic Properties of Three-dimensional Percolation Networks with Stretching and Bond-bending Forces", *Physical Review B,* in press (1988). (with S. Arbabi)

"Noise, Force Distribution and Multiscaling in Heterogeneous Elastic Media", submitted to *Physical Review Letters,* (April 1988). (with S. Arbabi)

"Statistical Physics of Linear and Nonlinear, Scalared Vector Transport Processes in Disordered Media", Proceedings of 3rd University of California Conference on Statistical Mechanics, in press (1988).

III. Theses Completed

"The Effect of Microscopic Inhomogenities on the Failure and Fracture Behavior of Disordered and Reinforced Materials", M. S. Thesis, M. D. Stephens, Department of Chemical Engineering, May 1988,

UNIVERSITY OF SOUTHERN CALIFORNIA

UNIVERSITY PARK • LOS ANGELES, CALIFORNIA 90089-0242

SCHOOL OF ENGINEERING
DEPARTMENT OF CIVIL ENGINEERING

February 4, 1988

Professor Hajime Matsuoka
Civil Engineering Department
Nagoya Institute of Technology
Gokiso-cho, Showa-Ku
Nagoya 466
Japan

Dear Professor Matsuoka:

As a follow-up to my visit of your laboratory in the Nagoya Institute of Technology in December 1987, I would like very much to explore your interest in collaborating with the Granular Group of the University of Southern California on the investigation of the micromechanical and physical behavior of granular materials.

The Granular Group is an interdisciplinary research team composed of four faculty members from three different engineering departments of the University of Southern California: Dr. Charles Campbell of Mechanical Engineering, Professor Joe Goddard and Dr. Mohammad Sahimi of Chemical Engineering, and myself in Civil Engineering. Our efforts are financially supported by the National Science Foundation and by the Air Force Office of Scientific Research.

One of our main research topics is the investigation of the changes of micromechanical and physical properties of granular media near failure; this type of problem is especially relevant to Japan and California where liquefied granular soils are responsible for most major catastrophes during earthquakes. It is worth pointing out that liquefaction analyses are current practice in Soil and Earthquake Engineering. However liquefaction is a complicated phenomenon which is not yet well understood nor investigated from a scientific point of view. Five pages were sufficient to summarize the past activity on micromechanics of granular material in the 240 page report entitled "Liquefaction of Soils during Earthquakes" compiled in 1985 by the Committee on Earthquake Engineering of the U.S. National Research Council.

The USC Granular Group would like to implement a collaborative research program with your Institute. However, since it is difficult to finance foreign exchanges with US funds, we must indicate that we are unable to provide you with travel support. I would like to suggest to you that you contact Japanese sources of funding such as the RIKEN Foundation. For your information I have attached some documentation on RIKEN. The study of the micromechanics of liquefying soils is certainly high technology research of vital interest to Japan and, therefore, worth funding by an organization such as RIKEN.

As the first step of our proposed collaboration, the granular group is interested in reanalyzing in more detail your experimental data on photoelastic measurement of contact forces in two-dimensional assemblages of araldite-B rods. We are particularly interested in describing the changes in the structures of force which percolate through granular assemblages. It is understood that you would be a co-author in all the publications involving your data. Should you be interested in implementing this collaborative program, we can define the terms of our exchange in further detail.

Looking forward to hearing from you in the near future.

Sincerely,

Jean Pierre Bardet

J.P. Bardet
Assistant Professor
Civil Engineering

JPB/swi

Encl.

APPENDIX

to

FINAL REPORT

on

RESEARCH

CRITICAL BEHAVIOR OF TRANSPORT AND MECHANICAL PROPERTIES IN PARTICULATE DISPERSIONS AND GRANULAR MEDIA

performed under

AFOSR Grant-87-0284

for the period

1 June 1987 - 31 May 1988

Submitted by

J. D. Goddard and C. Campbell
Co-Principal Investigators
University of Southern California

to

Major Steven C. Boyce
Program Manager
Directorate of Aerospace Sciences
Department of Air Force
Air Force Office of Scientific Research
Bolling Air Force Base, DC 20332-6448

15 September 1988

Critical Behavior of Transport and Mechanical Properties in Particulate Dispersions and Granular Media

Abstract

Following is a technical summary of research supported in part by AFSOR Grant-87-0284 on the mechanics and transport properties of granular materials. Part 1 (by J. D. Goddard and Y. M. Bashir) is a detailed account of research on certain aspects of the quasi-static mechanics, and Part 2 (by C. S. Campbell) provides a brief summary of published work on the mechanics and thermophysical properties of rapidly-sheared granular flows.

In Part 1, an extended summary is given of theory and 2D numerical simulations of dilatancy and stress in particle assemblies. The classical Reynolds theory is reformulated in continuum-mechanical terms, according to a new theory of internally constrained continua. This formulation allows for a consistent, invariant description of dilatancy in arbitrary deformation processes. Also, it reveals clearly the stress indeterminacy associated with the dilatancy constraint.

The above theory, cast in a form that is strictly valid only for isotropic system, is employed to interpret numerical simulations of the quasi-static simple shear of frictional disk assemblies. For 2D assemblies with equi-sized disks, it is found that the dilatancy (volumetric strain versus shear strain) is insensitive to particle friction, as has also been found in previous numerical simulations of certain other investigators. However, friction does appear to affect the degree of anisotropy, as reflected by the difference in normal stresses in the plane of shear. The high degree of anisotropy found in these idealized particle arrays, indicate the need for constitutive relations which account for anistropy in such systems.

Part 1

Quasi-Static Mechanics of Granular Media[1]

by

J. D. Goddard and Y. M. Bashir[2]

1 Reynolds Dilatancy

Dilatancy was first defined by Reynolds in 1885 [22] as *a definite change of the bulk consequent on a definite change of the shape.* The expansion of granular mass upon deformation is caused effectively by grains riding-up over each other to allow for shearing motions.

In his classic paper, Rowe [25] stressed the importance of accounting for dilatancy in any mechanical theory for granular materials and warned, with others [18], that ignoring dilation results in large differences between observations and calculations for deformation problems. Davis and Deresiewicz [7], Drescher and De Josselin De Jong [8], Christoffersen, Mehrabadi and Nemat-Nasser [5, 16], and Kishino [15] shared this view and tried to relate dilatancy to stress and deformation from microstructural considerations.

Rowe [24] considered regular arrays of both rods and spheres and gave a simple theory relating volumetric strain to axial strain, involving the angle of friction and a factor dependent on the geometry of the stack as the only parameters. Rowe's theory has been a subject of much controversy [1, 11, 14 ,17, 23, 27, 28, 31, 34]. Many have criticized the theory since it is based on a deformation mechanism that includes only sliding at contacts but does not take into account the effect of particle rotations.The importance of rotations was later tested experimentally by Oda , Koshini and Nemat-Nasser [20] and also stressed by Shwartz, Johnson and Feng [26] and by Cundall and Strack [6] in their simulations of flow of granular materials. The latter diminished the role of interparticle friction on dilation while Oda *et al.* believed that friction increases it.

[1]Exerpts from a paper in progress.

[2]Graduate Research Assistant.

From a physical point of view dilatancy appears essential to the correct description of a number of phenomena, including ***strain localization*** and ***soil liquefaction*** [2, 18, 29, 30, 33].

1.1 Extensions of the Reynolds Theory

Reynolds [22] assumed that in a state of maximum density of a collection of spherical particles, any contraction in one direction is accompanied by an equal extension at right angles in two other directions. In modern, tensor notation in terms of the principal values $\dot{\epsilon}_i$ strain-rate tensor $\mathbf{D}$, the Reynolds hypothesis becomes:

$$\dot{\epsilon}_2 = \dot{\epsilon}_3 = -\dot{\epsilon}_1 \tag{1}$$

The rate of volumetric strain, $\dot{\epsilon}_v$ is :

$$\dot{\epsilon}_v = tr(\mathbf{D}) = \dot{\epsilon}_1 + \dot{\epsilon}_2 + \dot{\epsilon}_3 = -\dot{\epsilon}_1 \tag{2}$$

so that equation (1) becomes:

$$\dot{\epsilon}_v = |\dot{\epsilon}_1| \tag{3}$$

In order to extend Reynolds' elemetary arguments to arbitrary states of deformation, we present below a generalization of the theory of internally constrained continua [35], in which allowance is now made for non-holonomic constraints, that is, constaints on kinemetics which are not generally derivable from constraints on static configurations.(This subject is well known in the classical mechanics of systems with finite degrees of freedom [19].)

As the simplest generalization of the Reynolds theory, in an invariant form applicable for any deformation, we write:

$$\dot{\epsilon}_v = \alpha\,|\mathbf{D}| \tag{4}$$

where:-

$$|\mathbf{D}| = tr(\mathbf{D}\cdot\mathbf{D})^{1/2} \tag{5}$$

or :

$$\dot{\epsilon}_v = \alpha(\dot{\epsilon}_1^2 + \dot{\epsilon}_2^2 + \dot{\epsilon}_3^2)^{1/2} \tag{6}$$

Using equation (1) with equation (6) yields:

$$\dot{\epsilon}_v = \alpha\sqrt{3}\,|\dot{\epsilon}_1| \tag{7}$$

The scalar quantity α, which we call the coefficient of dilatancy, may in general depend on the entire history of deformation of the granular mass. The classical strain-based (holonomic) theory of Reynolds produces a simple expression for α with a periodic dependence on strain and allows for compaction, $\alpha < 0$, as well as dilation, $\alpha > 0$. However, it is doubtful that Reynolds' elementary arguments would hold far from the state of maximum density. While Reynolds seemed to be thinking in terms of an isotropic structure, the state of maximum density for monosized spheres (3D) or disks (2D) corresponds in fact to hexagonal close-packed arrays which are mechanically *anisotropic*. Hence, there are some internal inconsistencies in his elementary arguments. At any rate his theory is seen by equations (3) and (7) to correspond to $\alpha = \sqrt{1/3}$ at the state of maximum density for spheres.

Here, we repeat Reynolds' argument in a form suitable for 2-dimensional arrays of equal circular disks or cylinders. Assuming a similar deformation mechanism, one can see from figure (1) that the ratio of the area A of the deformed triangle $a'b'c'$ to the area A_0 of the undeformed triangle abc, representing the two-dimensional volumetric strain ϵ_v, is given by:

$$\epsilon_v = \frac{A}{A_0} = \frac{H\sqrt{(2R)^2 - H^2}}{H_0\sqrt{(2R)^2 - H_0^2}} = \lambda_1\lambda_2 \tag{8}$$

Here:

$$\lambda_1 = \frac{H}{H_0}, \lambda_2 = \frac{\sqrt{(2R)^2 - H^2}}{\sqrt{(2R)^2 - H_0^2}}$$

are stretch ratios. For close-packed discs $H_0 = \sqrt{3}$ and thus $H = \sqrt{3}\lambda_1$. Therefore:

$$\lambda_2 = \sqrt{(2R)^2 - 3\lambda_1^2} \tag{9}$$

and

$$\epsilon_v = \lambda_1\sqrt{(2R)^2 - 3\lambda_1^2} \tag{10}$$

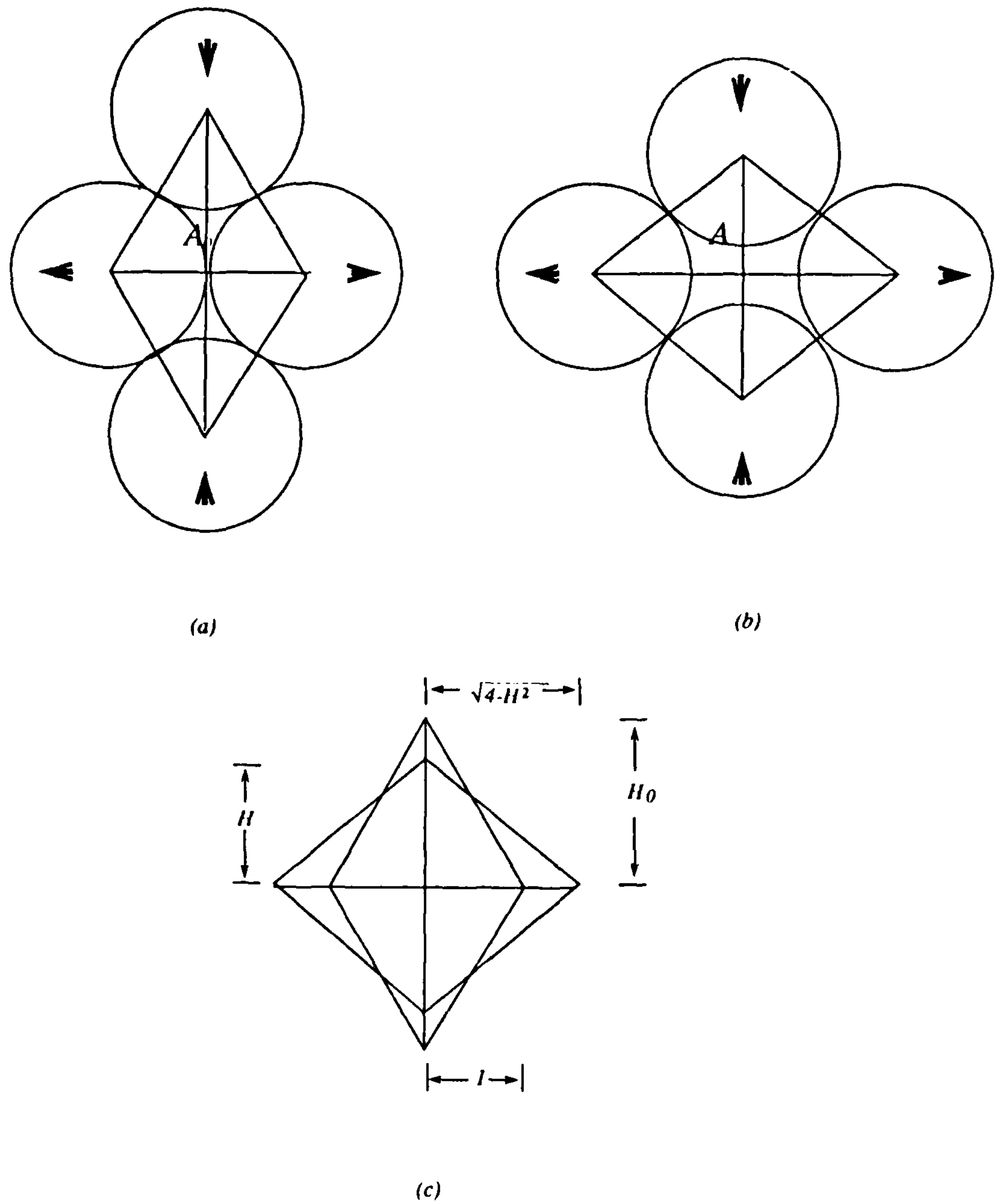


Figure 1: Deformation mechanism in 2-dimensional case.

Differentiating equation (10) with respect to time:

$$\dot{\epsilon}_v = \frac{1}{2}\lambda_1 \frac{-6{\lambda_1}^2\dot{\epsilon}_1}{\sqrt{(2R)^2 - 3\lambda_1^2}} + \lambda_1\dot{\epsilon}_1\sqrt{(2R)^2 - 3\lambda_1^2} \tag{11}$$

At the maximum density, *i.e.* at $\lambda_1 = 1$, equation (11) becomes:

$$\dot{\epsilon}_2 = \left(\frac{1}{2}\frac{-6\dot{\epsilon}_1}{(2R)^2 - 3\lambda_1}\right) = -3\dot{\epsilon}_1 \tag{12}$$

and

$$\dot{\epsilon}_v|_{\lambda_1=1} = -3\dot{\epsilon}_1 + \dot{\epsilon}_1 = -2\dot{\epsilon}_1 = 2\,|\dot{\epsilon}_1| \tag{13}$$

But:

$$|\mathbf{D}| = \left(\dot{\epsilon}_1^2 + \dot{\epsilon}_2^2\right)^{1/2} = \left(\dot{\epsilon}_1^2 + (3\dot{\epsilon}_1)^2\right)^{1/2} = \sqrt{10}\,|\dot{\epsilon}_1| \tag{14}$$

Therefore, from equations (13) and (14) one can obtain the following result for the 2-dimensional case:

$$\dot{\epsilon}_v = \frac{2}{\sqrt{10}}\,|\mathbf{D}| = \sqrt{\frac{2}{5}}\,|\mathbf{D}| \tag{15}$$

or $\alpha = \sqrt{\frac{2}{5}}$. The above reasoning is similar to that employed by Rowe [24], whose experiments on hexagonally close-packed spheres and rods give close agreement with the Reynolds theory near a state of maximum density.

To illustrate the application to simple shear involving a simultaneous planar isotropic expansion, we note that the x, y (1,2) components of $\mathbf{D}$ are given by :

$$\mathbf{D} = \frac{1}{2}\begin{pmatrix} \dot{\epsilon}_v & \dot{\gamma} & 0 \\ \dot{\gamma} & \dot{\epsilon}_v & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{16}$$

so that equation (4) reduces to a shearing dilation, with

$$s = \frac{d\epsilon_v}{d\gamma} = \frac{\dot{\epsilon}_v}{\dot{\gamma}} = \frac{\alpha}{(2-\alpha^2)^{1/2}} \tag{17}$$

Thus, it is seen by (15) that $s = 1/2$ for disks in 2D, whereas for equisized spheres in 3D one obtains from (4) $s = 1/\sqrt{5} = 0.447...$ for the expansive simple shear (16), and $s = \sqrt{3}/4 = 0.433...$ for simple shear with isotropic 3D expansion and $s = 1/(2\sqrt{2}) = 0.353...$ for a uniaxial compression.

Zhang and Cundall [37] in their computer simulation of 3-D systems of sphere found that the slope of the curve was approximately 1/3 compared to the Reynolds theory value of 0.353.... Given that their systems were not monosized spheres which Reynolds [22] assumed, the agreement is remarkable, a fact that appears to have been overlooked in [37]. It is also noteworthy that the slope of Zhang and Cundall's curve of volumetric strain versus shear strain was almost constant throughout the entire deformation range (up to shears of greater than 0.35) and not limited to the state of maximum density assumed by Reynolds [22] and Rowe [24].

1.2 Interpretation of Dilatancy via the Theory of Internal Constraints

We postulate here that an *internal material constraint* on the rate of deformation $\mathbf{D}$ can be represented by means of a second-rank symmetric tensor $\mathbf{N}$, in the form:

$$\mathbf{N} : \mathbf{D} \equiv tr(\mathbf{N} \cdot \mathbf{D}) \equiv N_{ij} D_{ij} = 0 \tag{18}$$

In six-dimensional vector space of strains, $\mathbf{N}$ may be viewed as the vector normal to a hyperplane (linear space) in which the strain rate $\mathbf{D}$ is required to lie, with, in general, each point in strain space through which a material point moves having a different hyperplane attached to it. In the usual holonomic theory [35] $\mathbf{N}$ is assumed to be derivable from a scalar constraint on strain, so that the hyperplane in question represents the local tangent space or linear 'support'. Standard examples are incompressible materials, where $\mathbf{N}$ is proportional to the unit tensor $\mathbf{1}(N_{ij} = const.\delta_{ij})$, or materials which are enextensible along certain material elements or 'fibers', in which case $\mathbf{N}$ is proportional to the dyadic or tensor product $\mathbf{ee}$ $(N_{ij} = const.e_i e_j)$, where $\mathbf{e}$ is a physical-space vector lying along the fiber direction.

In the case of a dilatant granular mass, the relation (4) can also be written in the form (18), with :

$$\mathbf{N} = a\mathbf{A} + b\mathbf{B} \tag{19}$$

where

$$\mathbf{A} = \alpha\hat{\mathbf{A}} - \mathbf{1} \quad (A_{ij} = \alpha\hat{D}_{ij} - \delta_{ij}) \tag{20}$$

$$\mathbf{B} = \alpha\hat{\mathbf{B}}^2 - (tr\hat{\mathbf{D}}^3)\mathbf{1} \quad (B_{ij} = \alpha\hat{D}_{ik}\hat{D}_{kj} - tr\hat{\mathbf{D}}^3\delta_{ij}) \tag{21}$$

a, b are arbitrary scalar constants, and

$$\hat{\mathbf{D}} = \frac{\mathbf{D}}{|\mathbf{D}|} = \frac{\mathbf{D}}{(tr\mathbf{D}^2)^{1/2}} \tag{22}$$

is the 'versor' or 'direction' of $\mathbf{D}$ in strain-rate space [12,13], in terms of which the constraint (4) becomes :

$$tr\hat{\mathbf{D}} \equiv \hat{\mathbf{D}} : \mathbf{1} = \alpha \tag{23}$$

With complex materials, one may anticipate that an internal constraint $\mathbf{N}$ may not always be derivable from functional restrictions on strain relative to a fixed state but rather may depend on the entire strain-path or strain-history of a material point, in which case we refer to $\mathbf{N}$ as a *non-holonomic* constraint. Because of their static particulate microstructure and their general tendency towards hysteretic behavior, we expect that dilatancy in the quasi-static motion of granular media should be treated as a non-holonomic constraint. While relations of the general form (4) and (18) can be derived from a constraint on the strain tensor representing a connection between volume and shape, it seems appropriate to allow for less restrictive forms in relations like (19), (20) and (23). Thus, the scalar parameter α or coefficient of dilatancy must be regarded in general as a *functional* depending on the entire strain history so the constraint is itself a rheological variable.

Work Principle

Whether holonomic or non-holonomic, the existence of internal constraints leads to rheologically indeterminate stresses [35], a fact which does not appear to be appreciated in much of the literature on soil mechanics and granular media. In particular, as a direct extension of an existing principle [35], one can state that, subject to the internal constraint (18), the stress tensor $\mathbf{T}$ may be specified rheologically only up to an additive stress $\mathbf{T}^\circ$, say, which *does no work* in any deformation compatible with the constraint. It follows that [35] $\mathbf{T}^\circ$ is given by :

$$\mathbf{T}^\circ = \lambda\mathbf{N} \tag{24}$$

where the constant of proportionality λ is a Lagrange multiplier that represents a force of reaction to the constraint. As with pressure p in and incompressible material ($\mathbf{N} \equiv \lambda\mathbf{1}, \lambda \equiv -p$) or the 'fiber tension' σ in an inextensible material ($\mathbf{N} \equiv \mathbf{ee}, \lambda \equiv \sigma$), the stress $\mathbf{T}^{\circ}$ in (24) reprenents a dynamical field variable which, not being determined by the material deformation, is governed instead by the momentum balance or equations of mechanical equilibrium together with applied external forces. Thus, the quantities λa and λb resulting from the substitution of an assumed representation like (19) into (24) would also have to be determined from the solution to a specific mechanical boundary-value problem.

To illustrate the above principle for the case of the representaion (19) and the planar sheared expansion of (16), we recall that:

$$\hat{\mathbf{D}} = \frac{\dot{\gamma}}{2}\begin{pmatrix} s & 1 \\ 1 & s \end{pmatrix}, \mathbf{T} = \begin{pmatrix} -p_{11} & \tau \\ \tau & -p_{22} \end{pmatrix} \tag{25}$$

with

$$p = -(p_{11} + p_{22})/2$$

where s is given by (17), while p denotes pressure and τ shear stress. A bit of algebra shows that the tensors $\mathbf{A}$ and $\mathbf{B}$ in (19) are linearly dependent in the planar case, so that the term in $\mathbf{B}$ may be discarded. Whence, it follows by (19) and (24) that:

$$\mathbf{T}^{\circ} = const. \begin{pmatrix} -1 & s \\ s & -1 \end{pmatrix} \tag{26}$$

That is, the indeterminate stress represents a stress state in which:

$$\tau = sp, \quad p_{11} = p_{22} = p \tag{27}$$

This becomes entirely transparent on recalling that the stress-work $\dot{W} = \mathbf{T} : \mathbf{D}$ is given by (25) as :

$$\dot{W} = \tau\dot{\gamma} - p\dot{\epsilon}_v = (\tau - sp)\dot{\gamma} \tag{28}$$

with the $\tau\dot{\gamma}$ representing shear ('shape') work and $p\dot{\epsilon}_v$ volume work. While independent for a constrained material, these are connected by the dilatancy relation $\dot{\epsilon}_v = s\dot{\gamma}$ for the dilatant material. Thus, that part of the stress which does the work of deformation is given by $\tau - sp$, so that any stress state of the form (27) is obviously workless.

As appreciated by Reynolds [22], and also by Rowe [24,25], the above arguments have interesting consequences for the quasi-static motion of granular materials composed of nearly rigid frictional particles, in which kinetic energy and elastic strain energy are negligible. In this case, it can be seen that all the energy input (28) must be accounted for by frictional dissipation associated with (Coulombic) sliding friction. Therefore, it follows that for the limiting case of ideal frictionless particles, (28) must vanish identically and the stress state or simple shear is of the form (27). That is, *all* stresses represent workless forces of reaction.

Based on the principle of internal constraint, which has apparently been unrecognized by Reynolds and subsequent workers, we can make certain very definite statements about the stress pattern for ideal frictionless systems once the form of the constraint $\mathbf{N}$ is known. For example, if the constraint is assumed to have the form (19)- (23), then the quasi-static stress in a frictionless particle system is given immediately by (24) for general deformations, which reduces to the form in $\mathbf{D}$ associated with the famous Reiner-Rivlin fluid model [12,13].

Because the Reiner-Rivlin model and the forms (19)- (23) are generally valid only for isotropic materials they may have limited validity for granular materials, except for certain special cases. For example, such forms may apply to initially isotropic states of particle arrays (such as random sphere packs) or to particulate systems involving highly irregular distributions of particle shapes and sizes. This a matter which we hope to clarify further in our future research and computer simulation. At the same time we are working out a parallel theory of internally-constrained materials which are assumed to develop anisotropy under deformation.

Some of the issues involved in this research would appear to be of crucial importance to the formulation of continuum rheological equations, for if the dilatancy and associated form of the constaint $\mathbf{N}$ are known in (18), then for any stress state $\mathbf{T}$ the rheologically determinate (frictional) stress $\mathbf{T}'$, say, is given generally by the *projection* onto the space normal to $\mathbf{N}$:

$$\mathbf{T}' = \mathbf{T} - (\mathbf{T} : \mathbf{N})\hat{\mathbf{N}} \equiv \mathbf{T} - tr(\mathbf{T} \cdot \mathbf{N})\hat{\mathbf{N}} \tag{29}$$

(which is the analog of deviatoric stress for incompressible materials) where:

$$\hat{\mathbf{N}} = \frac{\mathbf{N}}{|\mathbf{N}|} \tag{30}$$

is the versor of N. Viewed in these terms, the micromechanical energy-dissipation arguments of Rowe [24] and subsequent works take on a much more transparent meaning.

If attention is not paid to the role of dilatancy constraints in the formulation of constitutive equations, it is not clear to us that such equations would satisfy the basic thermodynamic restrictions inherent to the quasi-static deformation of frictional granular masses.

2 Numerical Simulations of 2D Cylinder Assemblies

We have developed our own computer program for the simulation of the quasi-static mechanics of granular assemblies, which ultimately we hope to 'benchmark' aginst existing codes such as the well-known 'TRUBALL' program of Cundall and co-workers [6,37]. While we have not studied the latter in full detail, our methods appear to be somewhat different. Although we adopt the same type of spatially periodic-cell model, which is already well known in molecular-dynamics and high-speed granular flow computations, our method of defining the 'fabric' or network of particle contact appears different and better adapted to large strains. Also, our method of solving the microscopic force balance appears somewhat different from previous works. In particular, we decompose the translation and rotation of each particle $(\mathbf{u}, \omega)$ into mean and 'fluctuating' parts $(\bar{\mathbf{u}}, \bar{\omega})$ and $(\mathbf{u}', \omega')$, say, the mean displacements being given by, in any small strain interval, by the macroscopically imposed strain increment, and the fluctuations being such as to satisfy the force and torque balance for each particle. This results in a quasi-linear system of equations

$$\mathbf{A} \cdot \mathbf{U}' = \mathbf{b} \tag{31}$$

where: $\mathbf{U}' = \left[\mathbf{u}'(\mathbf{1}), \omega'(1), \mathbf{u}'(\mathbf{2}), \omega'(2), ..., \mathbf{u}'(\mathbf{N}), \omega'(N)\right]$ is the collection of fluctuating displacements $\mathbf{U}'$ and rotations ω' for the N particles in a periodic cell, $\mathbf{A}$ is a 'grand stiffness matrix' determined by the elastic and frictional compliances of the paticle contancts, and $\mathbf{b}$ is the forcing associated with the imposed mean motion $\bar{\mathbf{U}}$.

2.1 Preliminary Numerical Results and Future Work

Figures (2)- (5) show some selected results from our numerical simulations, which were performed for simple linear elastic-contact model with a Coulomb (tangential) sliding friction. In particular, the normal and tangential forces between particles in contact are given by the relations of the form:

$$f_n = K_n \triangle u_n \tag{32}$$

$$f_t = \begin{cases} K_t \triangle u_t, & forY < 0 \\ \mu |f_n|, & forY \geq 0 \end{cases} \tag{33}$$

where:

$$Y = \mu |f_n| - K_t | \triangle u_t| \tag{34}$$

is a 'yield' function for slip, and $\triangle u_n$ and $\triangle u_t$ refer to suitably-defined relative normal and tangential particle displacements at the contact point. Here, K_n and K_t denote, respectively the normal and tangential elastic stiffness. While these are 'large' relative to external confining forces, corresponding to nearly rigid particles, their actual magnitudes are not crucial in our quasi-static systems since all (2D) stresses are scaled by K_n/R where R is a representative particle radius.

We have performed simulations for the simple shear of (25), for 2D periodic cells containing either 30, 56 or 120 particles (disks) of equal radius R. We present results here for the case of 56 particles. Figure (2) shows a representative set of configurations for shears, γ, ranging from zero to 0.25 (*i.e.*, 25 percent), starting from an initial density of 0.8978... obtained by slight expansion and randomization of a triangular close packing (density 0.907...). As seen from Figure (2) the sheared particle assembly gradually approaches a cubic (square) packing (density 0.785...) associated with the horizontal sliding of layers of particles.

In order to determine the shear dilatancy represented by the parameter s in equation (17) we have employed various strategies or algorithms for dilation of the sheared granular mass. In one strategy, 'local dilation', the mass is expanded to avoid some prespecified overlap of any two particles. In another, perhaps more physically realistic strategy, 'global dilation', we control an externally applied pressure, in effect by 'spring-loading' the system.

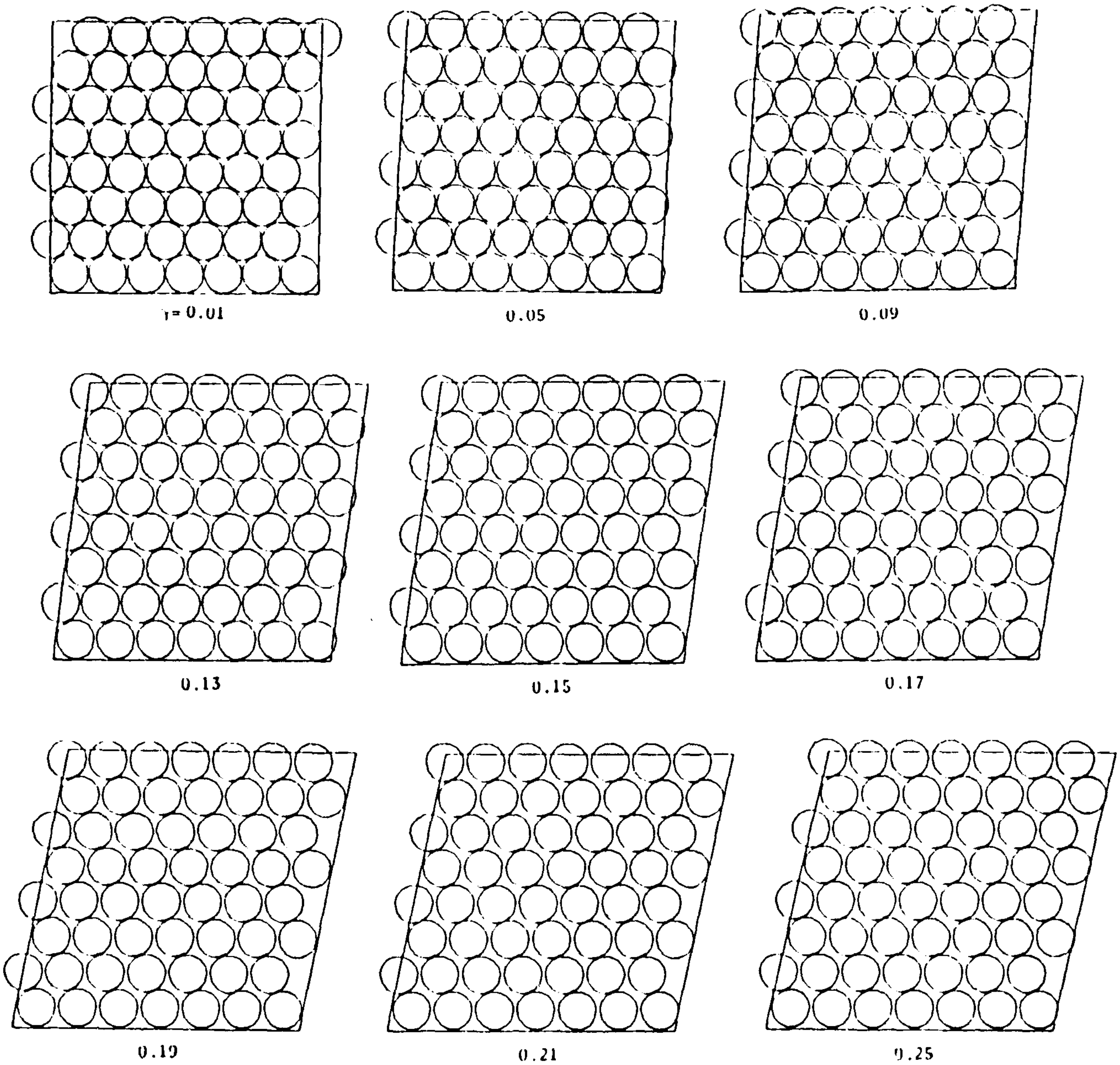


Figure 2: Representative configurations of the sheared system of particles at various shear-strain γ for friction coefficient $\mu = 0$.

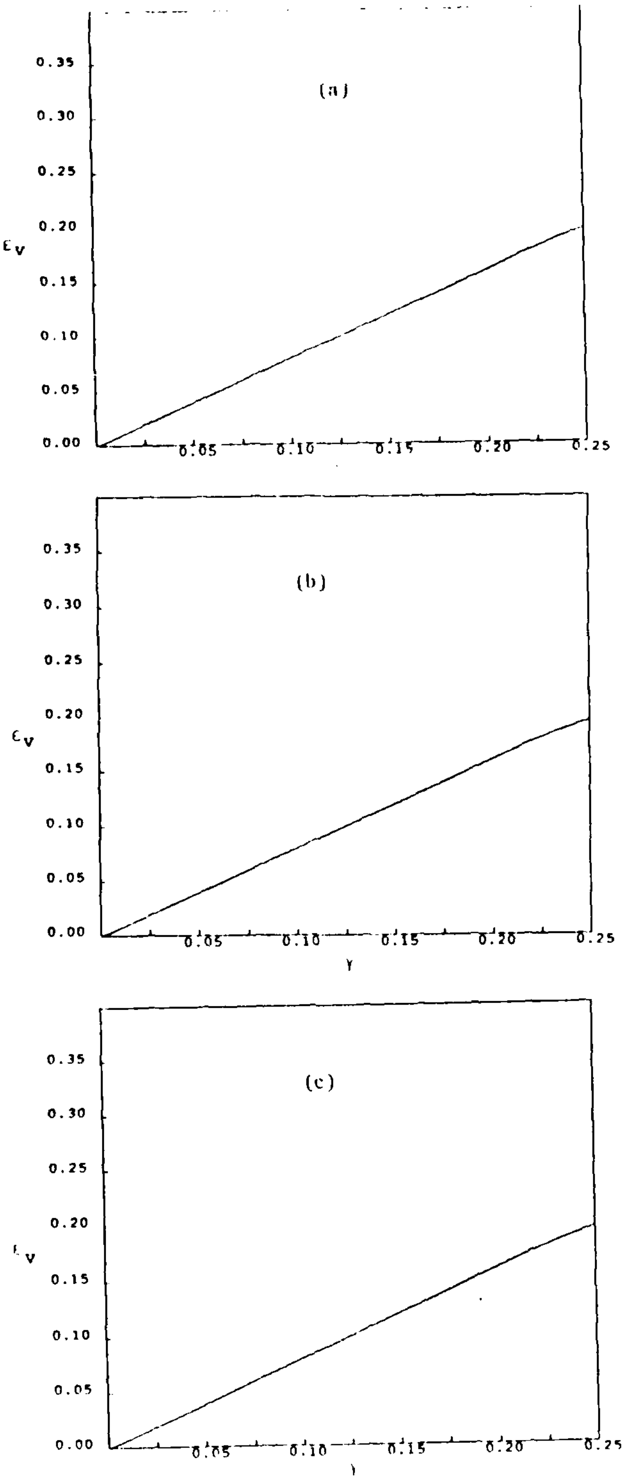


Figure 3: Volumetric strain ϵ_v versus shear-strain γ; (a) $\mu = 0$, (b) $\mu = 0.25$ and (c) $\mu = 0.5$.

Figures (3)- (6) show results for the global-dilation algorithm for an externally applied value of the pressure:

$$p = -\frac{1}{2}(T_{11} + T_{22}) \tag{35}$$

(where, in contrast to the usual soil-mechanics convention, our stress components T_{ij} are reckoned here as tensions.)

The computations in Figures (3)- (6) were carried out for a contact-stiffness ratio of $K_t/K_n = 0.8$, at three distinct sliding friction coefficients, $\mu = 0, 0.25$ and 0.50 (representing angles of internal friction $0°, 14°$ and $26.6°$, respectively), and for a control pressure $p = 10^{-6}$.

From the computations and the plot of volumetric (areal) expansion $\epsilon_v \equiv A/A_0 - 1$ in Figure (3), one concludes that the shearing dilatancy is given by $s \doteq 0.8$, independent of the sliding friction μ. The lack of dependence on μ corresponds to the findings of others in small strain simulations [6]. On the other hand, for the less realistic local-dilation algorithm our computations (not shown here) give a value of s close to the Reynolds theory, $s = 0.5$. We note from Figure (3) that at $\gamma = 0.25$, ϵ_v exceeds slightly the value of 0.144... associated with expansion from the initial density (0.8978...) to that associated with a cubic (square) array of disks (0.785...).

Figures (4) and (5) present the stress ratios:

$$\tau'/p = \tau/p - s \tag{36}$$

where $\tau \equiv T_{12} = T_{21}$ is the shear stress, and

$$N = (T_{11} - T_{22})/p \tag{37}$$

The stress τ' is of course that defined in equation (28) and represents the work done against friction. The small but non-zero values for $\mu = 0$ in Figure (4-a) represents small inaccuracies in the numerical calculations. Figures (4-b) and (4-c) show the effect of μ on τ', the increase with friction shown in 4(a)-4(b) being quite reasonable on physical grounds. As far as we know, past investigators have not made similar checks on the energy consistency of their numerical simulations.

The stress ratio N in equation (37) represents the effect of anisotropy in the particle assembly, since this quantity must vanish identically for isotropic systems (in accordance with the Reiner-Rivlin model discussed above). Thus, although friction has little effect on the dilatancy s, it appears to reduce the anisotropy reflected in N, as shown in Figure (5).

Finally, in an attempt to interpret our results in terms of particle contacts, we have computed the quantity

$$f = \frac{n}{6n_0} \tag{38}$$

where n =number of particle contacts, and n_0 =number of particles. The denominator $6n_0$ in (38) represents the maximum possible number of contacts for a triangular close-packed array, so that (38) represents the fraction of 'bonds' active in a 'network' of particle contacts. Since we suspect that such a criterion might be fruitfully employed to represent the well-known phenomenon of 'bridging' or 'arching' in granular masses, we have computed particle contacts at each shear step $\triangle\gamma$ in our computaions.

As seen by Figure (6), f lies below the critical value of $f_c = 0.347...$ [32] for *percolation* on a triangular network, which is what one would expect for a 'fluid-like' state of a continuously deforming system. If one modifies the ratio (38) by replacing $6n_0$ by $4n_0$ to obtain a value appropriate to a square lattice, which appears more representative of the fully expanded system, the resultant values of f still lie well below the percolation threshold $f_c = 0.5$ for square networks [32]. Thus, in either case we conclude that the particle-contact density lies below that of the 'solid' state associated with force percolation through static particle assemblies.

As future work we intend to perform multiple realizations of our shear simulations. Also, we propose to investigate several other questions, including:

1. scalar (electrical or thermal) conductivity of sheared assemblies,
2. effects of body forces (gravity),
3. hysteresis effects in cyclic shear,
4. polydispersity (multiple particle sizes), and
5. 3D simulations of granular masses.

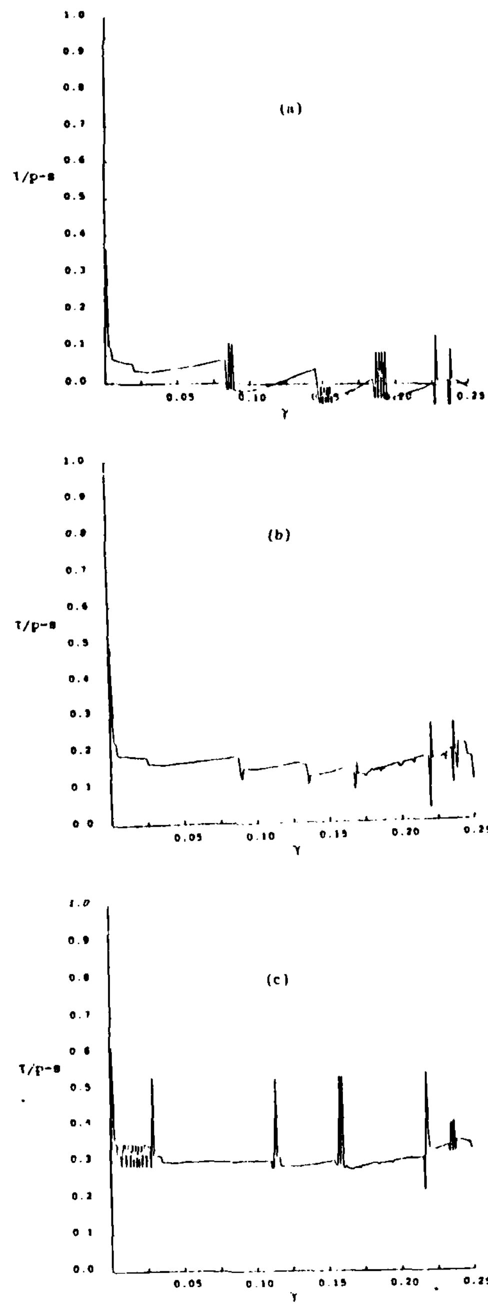


Figure 4: The stress ratio τ'/p versus shear-strain γ; (a) $\mu = 0$, (b) $\mu = 0.25$ and (c) $\mu = 0.5$.

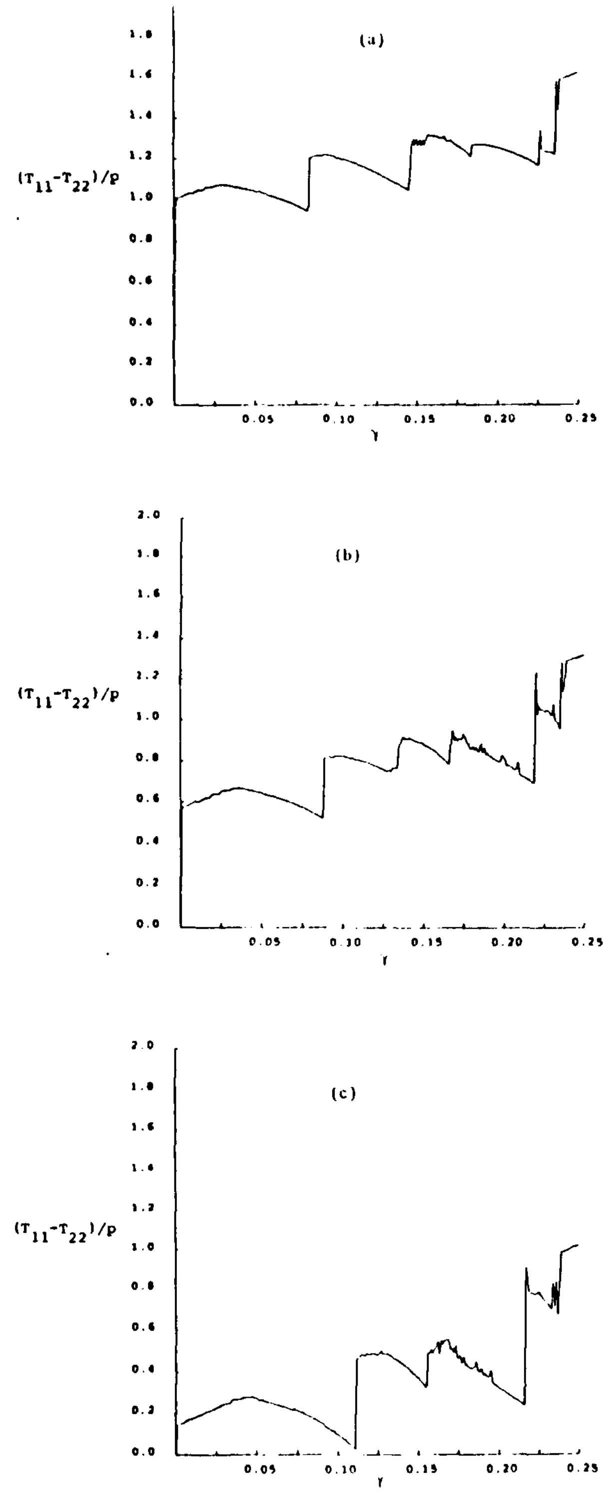


Figure 5: $N/p = (T_{11} - T_{22})/p$ versus shear-strain γ; (a) $\mu = 0$, (b) $\mu = 0.25$ and (c) $\mu = 0.5$.

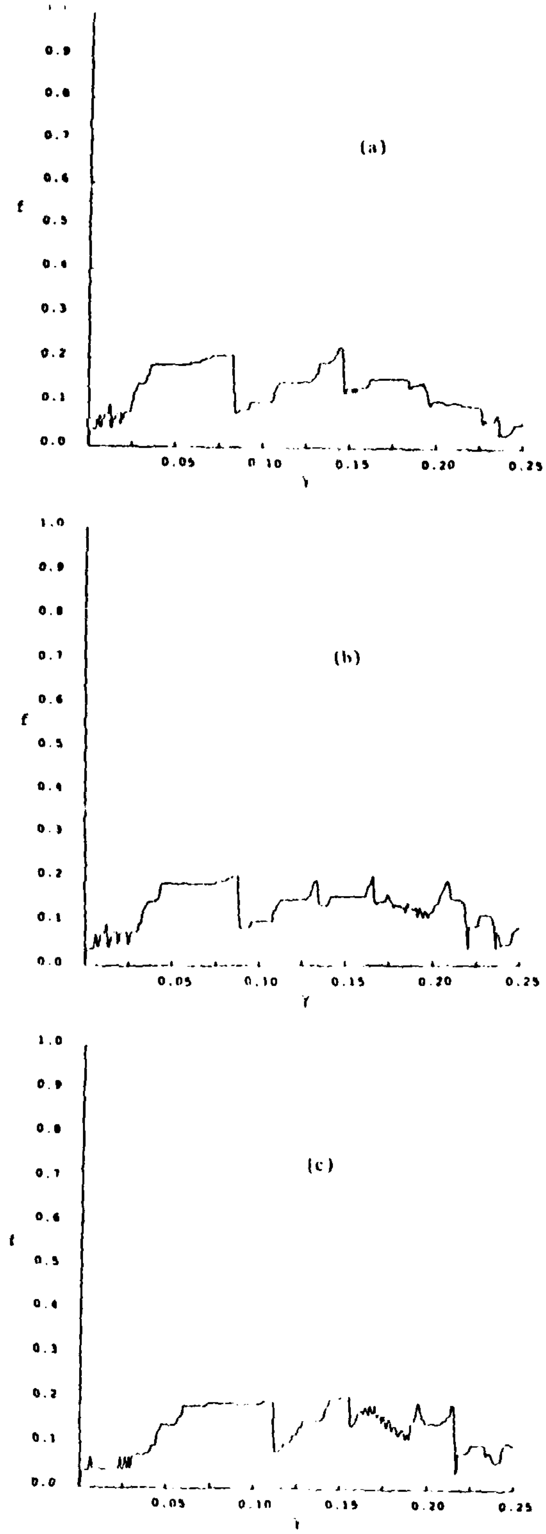


Figure 6: The fraction f of active contacts versus shear-strain γ; (a) $\mu = 0$, (b) $\mu = 0.25$ and (c) $\mu = 0.5$.

Part 2

Transport Processes in Rapid Granular Flows

by

C. S. Campbell

The main focus of this work is the study of the relationship between the mechanics and thermophysical properties of particulate materials subject to rapid shearing. Following is a summary of the research.

3 Particulate rotation as a heat transfer mechanims

The vorticity in shear flow causes spherical particles to rotate with an angular velocity of equal to about one-half the local shear-rate. Computer simulations have shown this to be as true for granular materials as it is for suspended particles in flowing fluids. We believe that this rotation can cause the transport of heat and therefore affect the heat transfer to any granular shear flow. The reasoning is as follows: The surface of the rotating particle will absorb heat on the hot side of the gradient and reject it on the cool side, causing a convective transport of heat within the particle. To gain a handle on the importance of this mechanism we have performed a theoretical analysis of a single particle rotating in an infinite stationary medium. In paper [36] we solve the problem exactly and compute the apparent conductivity enhancement due to the particle rotation. As perhaps the most important result we find that in the limit of large rotational Peclet number the system approaches the behavior of a single infinitely conductive particle. Thus, rotations would have very little effect for particles in air where the conductivity ratio is already quite large. This is apparent both in the isotherms generated from the exact solution and the calculated effective conductivity of the composite material. Less apparent is the appearance of anisotropy in the conductivity tensor at moderate Peclet number. However, the anisotropy disappears both as $Pe \to 0$ and as $Pe \to \infty$ where the solution approaches the equivalent Maxwell (non-rotating particle) solution for the zero-conductivity and infinite-conductivity particle respectively.

4 Effective conductivity in particle shear flows

The general goal here is to understand the mechanical enhancement of thermophysical transport in granular materials. Here the apparent conductivity of a granular material is determined while the material is sheared in an annular shear cell. (This is the completion of the work that originally engendered the above particle-rotation study.) The preliminary results of this work indicate that in simple shear flow the effective conductivity increases linearly with shear-rate. This is particularly satisfying as it has long been known that the effective viscosity of a sheared granular material also increases linearly with the shear-rate, indicating a certain internal unity in the two transport mechanisms. The key seems to lie in the so-called granular temperature which is a measure of the energy contained in the random motion of the particles. Computer simulations have shown that in a simple shear flow the granular temperature increases with the square of the shear-rate. This means that both the viscosity and the thermal conductivity in simple shear flow of a granular material vary as the square root of the granular temperature as predicted by kinetic theory for the dependence of both viscosity and thermal conductivity on the thermodynamic temperature. (This type of behavior should be expeccted from any rigid sphere system.) These preliminary results suffer from uncertainties about the experimental apparatus, as possible effects of conduction through the side walls could give rise to a large apparent thermal conductivity, (although we are quite content that the trends in the experiments are correct.) Unfortunately, the geometry of our shear cell is fixed by the necessity of maintaining good mechanical contact with the particles in order to drive the shearing motion. In work which is still continuing, our approach is to calibrate the apparatus by measuring materials of known conductivity and using he results to correct the conductivity measurements.

5 Work on basic mechanisms of high-speed granular flows

The AFSOR grant has also allowed completion oi two papers on this subject. The first [3] is part of a comprehensive computer simulation of the effects of boundaries on granular flows. This was originally begun to guide the design of wall boundaries for the heat transfer experiment described above in (3). We find that for frictional particles, couple stresses become very important in the neighborhood of boundaries in those cases where the boundary is likely to induce significant rotation in the particles. To our knowledge, it is the first paper ever to assess the importance of couple stresses. The second paper [4] analyzes anomalous land-slides that appear to travel with extremely low friction. Using three examples, it is shown that the low apparent friction can be accounted for solely by the particle mechanics, in distinct contrast to previous theories which invok extraneous mechanisms such as thin lubricating films of air or water.

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